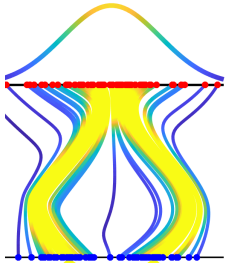
Machine Learning $\leftrightarrow$ Optimal Transport

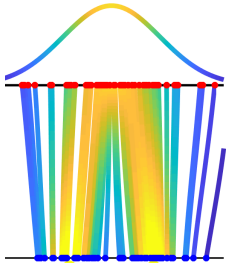
Old solutions to new problems and vice versa

Lars Ruthotto
Departments of Mathematics and Computer Science, Emory University
lruthotto@emory.edu
@lruthotto

Agenda: Machine Learning meets Optimal Transport

- **ML → OT: New Tricks from Learning**
  - based on relaxed dynamical optimal transport
  - combine macroscopic / microscopic / HJB equations
  - neural networks for value function
  - combine analytic gradients and automatic differentiation
  - generalization to mean field games and control problems
- **OT → ML: Learning from Old Tricks**
  - variational inference via continuous normalizing flows
  - applications: density estimation, generative modeling
  - OT $\rightsquigarrow$ uniqueness and regularity of dynamics
  - HJB, solid numerics, and efficient implementation
  - orders of magnitude speedup training and inference



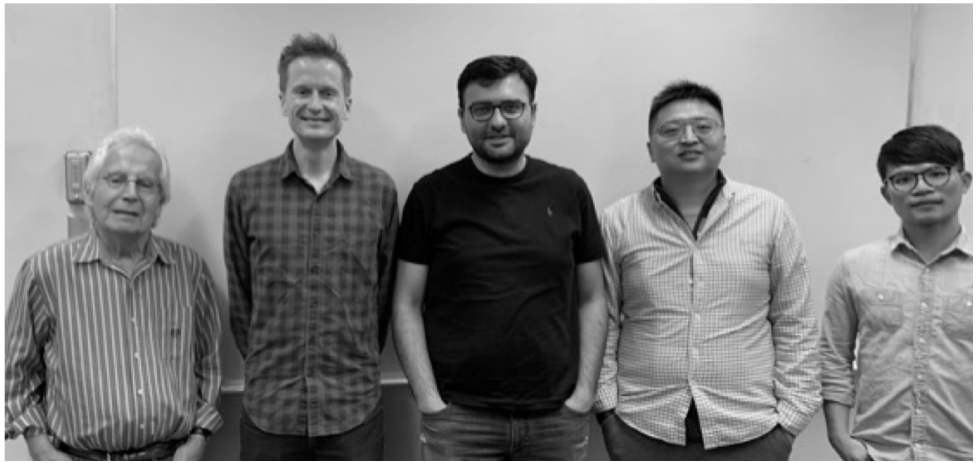


LR, S Osher, W Li, L Nurbekyan, S Wu Fung
A ML Framework for Solving High-Dimensional MFG and MFC
PNAS 117 (17), 9183-9193, 2020

D Onken, S Wu Fung, X Li, LR
OT-Flow: Fast and Accurate CNF via OT
arXiv:2006.00104, 2020.

A Machine Learning Framework for High-Dimensional OT (and more)

Team and Acknowledgements



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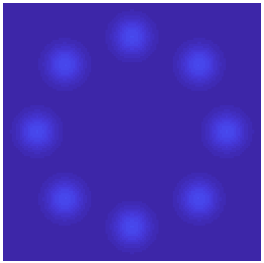
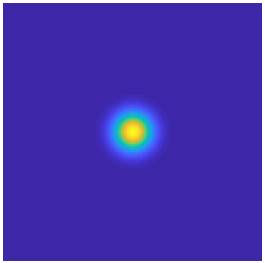
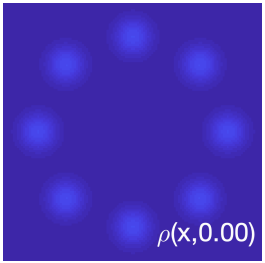
Special thanks: Organizers and staff of IPAM Long Program MLP 2019.



initial density, ρ_0



target density, ρ_1



density evolution

Dynamic Optimal Transport (Benamou and Brenier, '00)

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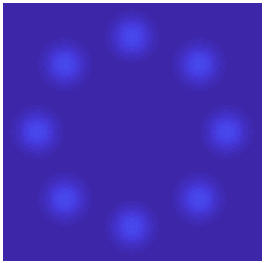
$$\begin{aligned} \text{minimize}_{v,\rho} \quad & \int_0^1 \int_\Omega \frac{1}{2} \|v(x,t)\|^2 \rho(x,t) dx dt \\ \text{subject to} \quad & \partial_t \rho + \nabla \cdot (\rho v) = 0, \quad \rho(\cdot, 0) = \rho_0(\cdot), \quad \rho(\cdot, 1) = \rho_1(\cdot) \end{aligned}$$



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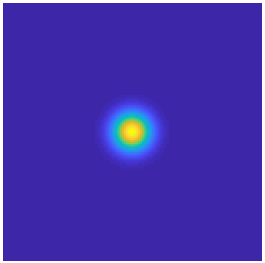

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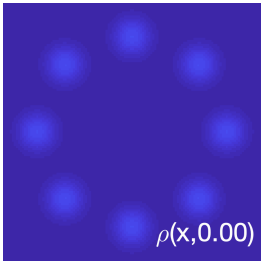

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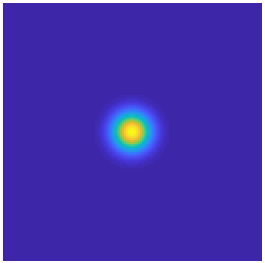

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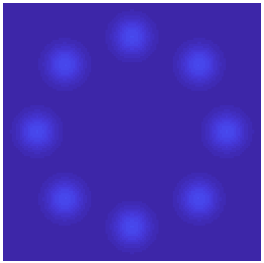

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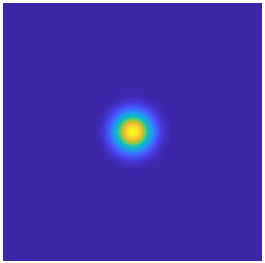

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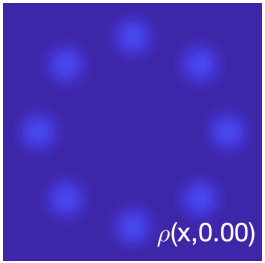


density evolution

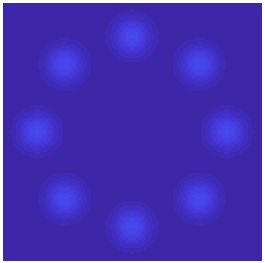
Relaxed Dynamical Optimal Transport

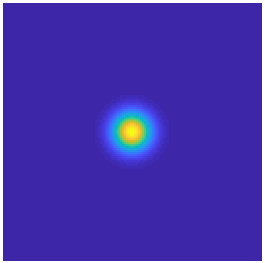
Given the initial density, ρ_0, and the target density, ρ_1, find the velocity v that minimizes the discrepancy between the push-forward of ρ_0 and ρ_1 and the transport costs, i.e.,

$$\begin{aligned} &\text{minimize}_{v,\rho} \mathcal{J}_{\text{MFG}}(\rho, v) \overset{\text{def}}{=} \int_0^1 \int_\Omega \frac{1}{2}\|v(x,t)\|^2 \rho(x,t) dx dt + \mathcal{G}(\rho(\cdot,1), \rho_1) \\ &\text{subject to} \quad \partial_t \rho + \nabla \cdot (\rho v) = 0, \quad \rho(\cdot,0) = \rho_0(\cdot) \end{aligned} \tag{CE}$$

Examples for terminal cost $\mathcal{G}$: L_2, Kullback Leibler divergence,...

Take away: relaxed OT problem is a potential mean field game (MFG)


initial density, ρ_0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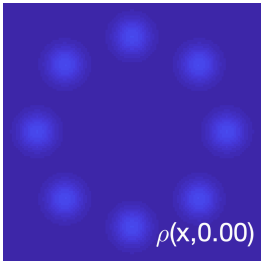

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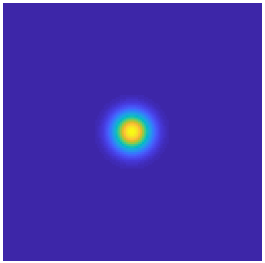
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Relaxed OT: A Microscopic View

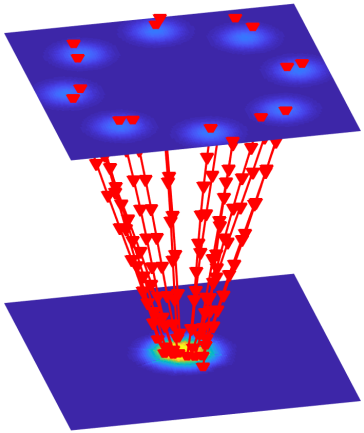
A single agent with initial position $x \in \Omega$ aims at choosing v that minimizes

$$J_{x,0}(v) = \int_0^1 \frac{1}{2}\|v(s)\|^2 ds + G\left(z(1), \rho(z(1), 1)\right),$$

where their position changes according to

$$\partial_t z(s) = v\left(s\right), \; 0 \le s \le 1, \quad z(0) = x.$$

- $G(x, \rho) = \frac{\delta \mathcal{G}(\rho, \rho_1)}{\delta \rho}(x)$ (variational derivative of $\mathcal{G}$)
- agent interacts with the population through ρ and G
- $z(\cdot)$ is characteristic curve of (CE) starting at x



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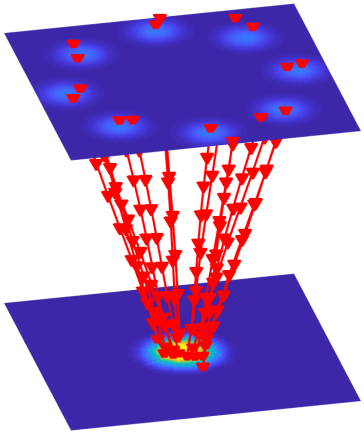
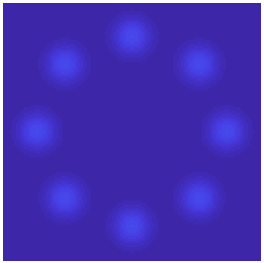
Useful to define the value of an agent's state (x, t) as

$$\Phi(x, t) = \inf_v J_{x,t}(v)$$



Hamilton-Jacobi-Bellman (HJB) Equation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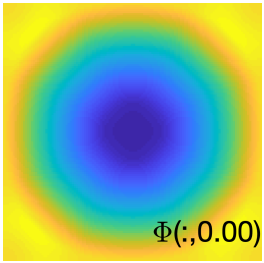
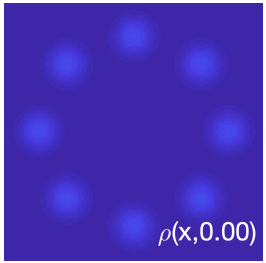
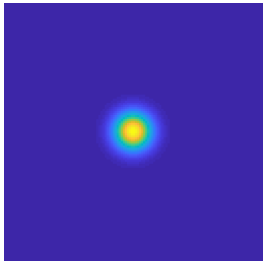


value function



density evolution


target density, ρ_1

Lasry & Lions '06: First-order optimality conditions of relaxed OT are

$$-\partial_t \Phi(x,t) + \frac{1}{2}\|\nabla \Phi(x,t)\|^2 = 0, \qquad \Phi(x,1) = G(x,\rho(x,1)) \tag{HJB}$$

and optimal strategy is $v(x,t) = -\nabla \Phi(x,t)$, which gives

$$\partial_t \rho(x,t) - \nabla \cdot (\rho(x,t)\nabla \Phi(x,t)) = 0, \quad \rho(x,0) = \rho_0(x) \tag{CE}$$

challenge: forward-backward structure and high-dimensional PDE

Machine Learning for High-Dimensional OT: Overview

Three options for solving the problem

1. minimize $\mathcal{J}_{\text{MFG}}$ w.r.t. (ρ, v), or $(\rho, -\nabla\Phi)$ (variational problem)
2. minimize $J_{x,t}$ w.r.t. v or $-\nabla\Phi$ for some points x (microscopic view)
3. compute value function by solving (HJB) and (CE) (high-dimensional PDEs)

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Idea: Combine advantages of the above to tackle curse of dimensionality

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Idea: Combine advantages of the above to tackle curse of dimensionality

- formulate as variational problem. minimize $\mathcal{J}_{\text{MFG}}(\rho, -\nabla\Phi)$
- eliminate (CE) with Lagrangian PDE solver $\rightsquigarrow$ 🌞 mesh-free, parallel
- parameterize Φ with NN $\rightsquigarrow$ 🌞 universal approximator, mesh-free, cheap(?)
- penalize violations of (HJB) $\rightsquigarrow$ 🌞 regularity, global convergence(?)

Lagrangian Method

Lagrangian Method for Continuity Equation

Assume Φ given. Then, the solution to

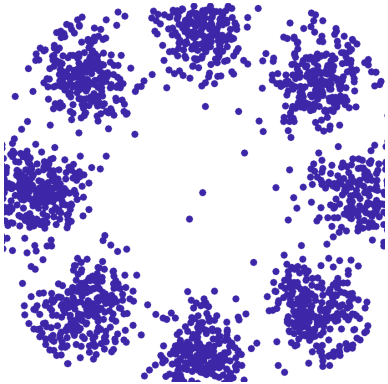
$$\partial_t \rho(x,t) - \nabla \cdot (\rho(x,t) \nabla \Phi(x,t)) = 0, \quad \rho(x,0) = \rho_0(x)$$

satisfies

$$\rho(z(x,t),t) \det \nabla z(x,t) = \rho_0(x)$$

along the characteristic curve

$$\partial_t z(x,t) = -\nabla \Phi(z(x,t)), \quad z(x,0) = x.$$



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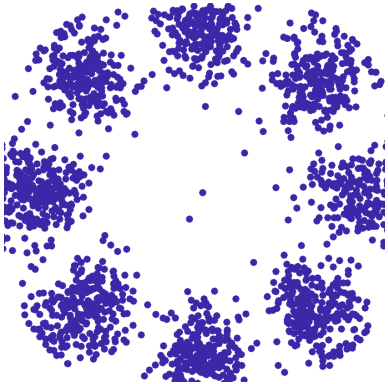

🔆🔆 instead of computing $\det \nabla z(x,t)$ (cost $\mathcal{O}(d^3)$ flops) use

$$l(x,t) \overset{\text{def}}{=} \log \det(\nabla z(x,t)) = \int_0^1 \Delta \Phi(z(x,t),t) dt$$

Hint: Compute z and l in one ODE solve (parallelize over $x_1, x_2, \ldots$).

Lagrangian Method for Optimal Transport

$$\begin{aligned}
\text{minimize}_{\Phi} \quad & \mathbb{E}_{\rho_0}\left[c_{\mathrm{L}}(x,1) + G(z(x,1)) + \alpha_1 c_{\mathrm{H}}(x,1) + \alpha_2 \|\Phi(z(x,1),1) - G(z(x,1))\|\right] \\
\text{subject to} \quad & \partial_t \begin{pmatrix} z(x,t) \\ l(x,t) \\ c_{\mathrm{L}}(x,t) \\ c_{\mathrm{H}}(x,t) \end{pmatrix} = \begin{pmatrix} -\nabla\Phi(z(x,t),t) \\ -\Delta\Phi(z(x,t),t) \\ \frac{1}{2}\|\nabla\Phi(z(x,t),t)\|^2 \\ \left|\partial_t\Phi(z(x,t),t) + \frac{1}{2}\|\nabla\Phi(z(x,t),t)\|^2\right| \end{pmatrix}, \quad t \in (0,1] \\
& z(x,0) = x, \quad l(x,0) = c_{\mathrm{L}}(x,0) = c_{\mathrm{H}}(x,0) = 0
\end{aligned}$$

Lagrangian Method for Optimal Transport

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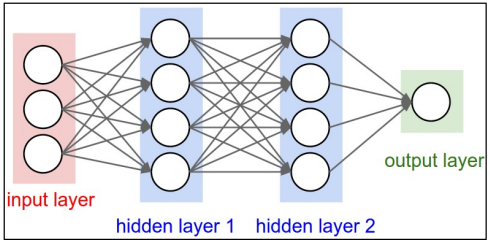
\end{aligned}
$$

- z and $l = \log\det$ needed to solve continuity eq. (CE)
- c_{L} and c_{H} accumulate cost along characteristic
- α_1, α_2: penalty parameters for HJB violation
- discretize dynamics with n_t steps of Runge-Kutta-4
- discretize $\mathbb{E}$ with Monte Carlo
- can use SA (SGD, ADAM,...) or SAA (BFGS, Newton,...) methods
- no grid needed and computation can be parallelized over x

Next, parameterize Φ with NN. Needed: $\nabla\Phi$ and $\Delta\Phi$

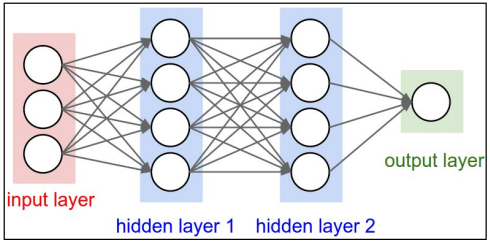
Neural Network Model

Deep Learning Revolution (?)



- deep learning: use neural networks (from $\approx$ 1950's) with many hidden layers
- able to "learn" complicated patterns from data
- applications: classification, face recognition, segmentation, driverless cars, ...
- recent success fueled by: massive data sets, computing power
- A few recent references:
  - Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17
  - **A radical new neural network design could overcome big challenges in AI**, MIT Tech Review '18

Deep Learning Revolution (?)



$$\begin{cases} \mathbf{Y}_{j+1} &= \sigma(\mathbf{K}_j\mathbf{Y}_j + \mathbf{b}_j) \\ \mathbf{Y}_{j+1} &= \mathbf{Y}_j + \sigma(\mathbf{K}_j\mathbf{Y}_j + \mathbf{b}_j) \\ \mathbf{Y}_{j+1} &= \mathbf{Y}_j + \sigma\left(\mathbf{K}_{j,2}\sigma(\mathbf{K}_{j,1}\mathbf{Y}_j + \mathbf{b}_{j,1}) + \mathbf{b}_{j,2}\right) \\ &\vdots \end{cases}$$

(Notation: $\mathbf{Y}_j$: features, $\mathbf{K}_j, \mathbf{b}_j$: weights, σ : activation)

- deep learning: use neural networks (from $\approx$ 1950's) with many hidden layers
- able to "learn" complicated patterns from data
- applications: classification, face recognition, segmentation, driverless cars, ...
- recent success fueled by: massive data sets, computing power
- A few recent references:
  - Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17
  - **A radical new neural network design could overcome big challenges in AI**, MIT Tech Review '18

Neural Network Model for Value Function

Let $s = (x, t) \in \mathbb{R}^{d+1}$ and use (NN + quadratic) model for value function

$$\Phi(s, \theta) = w^\top N(s, \theta_N) + \frac{1}{2} s^\top A s + c^\top s + b, \quad \theta = (w, \theta_N, \mathrm{vec}(A), c, b)$$

$N(s, \theta_N)$ is an M-layer ResNet with weights $\theta_N = (\mathrm{vec}(K_0), \ldots, \mathrm{vec}(K_M), b_0, \ldots, b_M)$.

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forward propagation:

$$\begin{aligned}
u_{-1} &= s \\
u_0 &= \sigma(K_0 u_{-1} + b_0) \\
u_1 &= u_0 + h\sigma(K_1 u_0 + b_1) \\
&\vdots \qquad\qquad \vdots \\
u_M &= u_{M-1} + h\sigma(K_M u_{M-1} + b_M),
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$$\begin{aligned} z_{M+1} &= w \\ z_M &= z_{M+1} + hK_M^\top \mathrm{diag}(\sigma'(K_M u_{M-1} + b_M)) z_{M+1}, \\ &\vdots \qquad\qquad \vdots \\ z_1 &= z_2 + hK_1^\top \mathrm{diag}(\sigma'(K_1 u_0 + b_1)) z_2, \\ z_0 &= K_0^\top \mathrm{diag}(\sigma'(K_0 s + b_0)) z_1, \end{aligned}$$

Output: $z_0 = \nabla_s (w^\top N(s, \theta_N))$

Next: Compute $\Delta\Phi(s, \theta) = \mathrm{tr}\left(E^\top (\nabla_s^2 (N(s, \theta_N) w) + A) E\right)$,

Computing the Laplacian of Value Function

$$\Delta\Phi(s,\theta) = \operatorname{tr}\left(E^\top(\nabla_s^2(N(s,\theta_N)w) + A)E\right) \quad \text{for} \quad E = \texttt{eye(d+1,d)}$$

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Second term trivial. Focus on NN part and use forward mode for first layer

$$\begin{aligned} t_0 &= \operatorname{tr}\left(E^\top \nabla_s (K_0^\top \operatorname{diag}(\sigma''(K_0 s + b_0))z_1)E\right) \\ &= (\sigma''(K_0 s + b_0) \odot z_1)^\top ((K_0 E) \odot (K_0 E))\mathbf{1}, \end{aligned}$$

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Get $\Delta(N(s,\theta_N)w) = t_0 + h\sum_{i=1}^M t_i$ where for $i \geq 1$

$$\begin{aligned} t_i &= \operatorname{tr}\left(J_{i-1}^\top \nabla_s(K_i^\top \operatorname{diag}(\sigma''(K_i u_{i-1}(s) + b_i))z_{i+1})J_{i-1}\right) \\ &= (\sigma''(K_i u_{i-1} + b_i) \odot z_{i+1})^\top((K_i J_{i-1}) \odot (K_i J_{i-1}))\mathbf{1}. \end{aligned}$$

Here, $J_{i-1} = \nabla_s u_{i-1}^\top \in \mathbb{R}^{m\times d}$ is a Jacobian matrix (update during forward pass)

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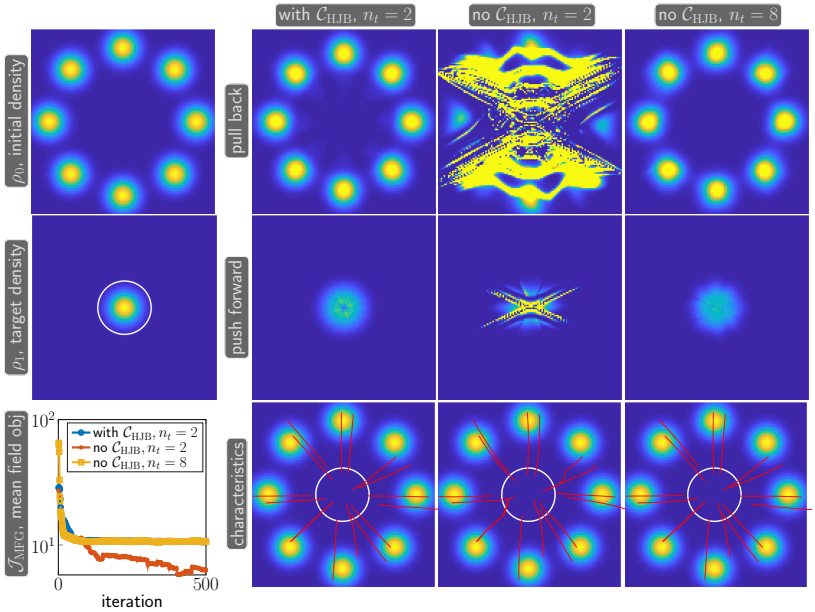
overall cost when $K_0 \in \mathbb{R}^{m\times(d+1)}$ is $\mathcal{O}(m^2 \cdot d)$ FLOPS

Numerical Experiments

Experiment 1: Benefit of HJB Penalty



HJB penalty improves accuracy and(!) lowers computational costs

Experiment 3: Comparison with Eulerian Solver

Eulerian scheme:

- dynamical OT formulation
- conservative finite volume
- leads to convex optimization
- solved to high accuracy with Newton's method

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A Multilevel Method for the Solution of Time Dependent Optimal Transport,
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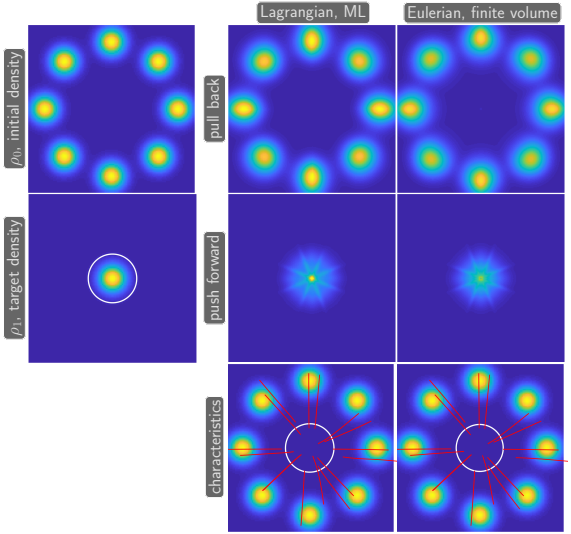
Comparison:

	# parameters	$\mathcal{J}_{\text{MFG}}$
Eulerian, fine	3,080,448	1.066e+01 (100.00%)
Eulerian, coarse	376,960	1.082e+01 (101.47%)
MFGnet ($n_t = 2$)	637	1.072e+01 (100.59%)
MFGnet ($n_t = 8$)	637	1.063e+01 (99.69%)



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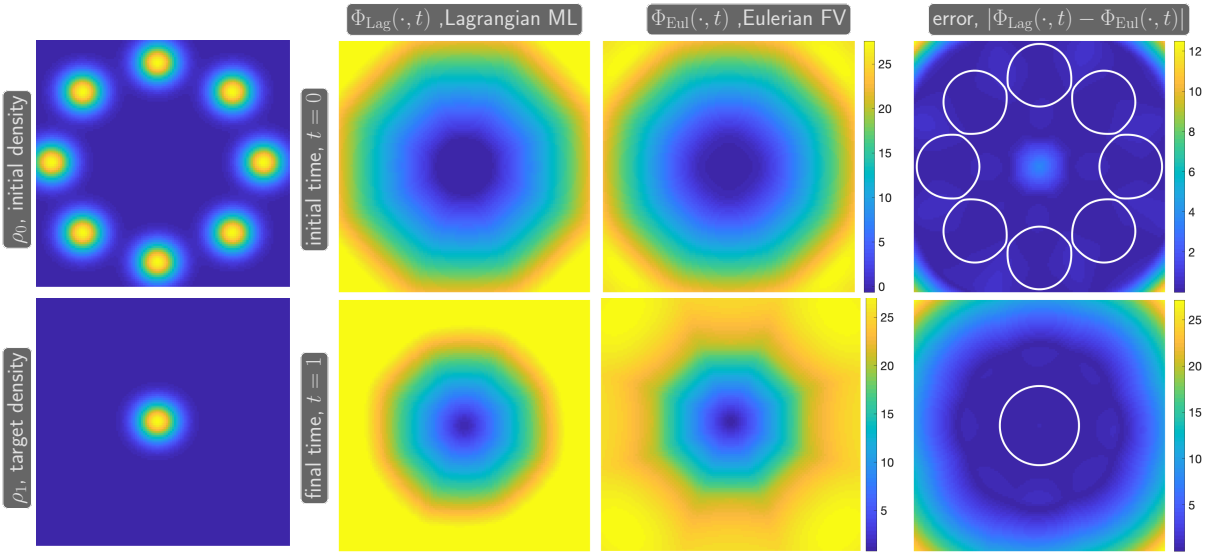
Experiment 3: Comparison of Value Functions



Take away: Eulerian ($\approx$ 3M parameters) and Lagrangian-ML (637 parameters) give comparable accuracy.

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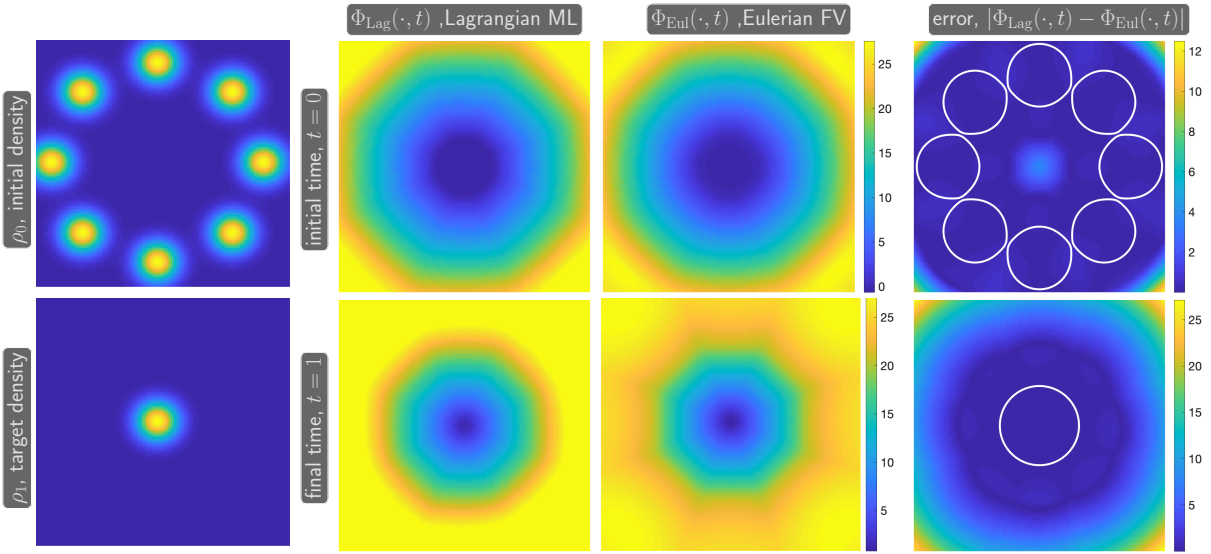

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Extension: Mean Field Games / Mean Field Control

Model large populations of rational agents playing non-cooperative differential game.

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$$\text{minimize}_{v,\rho}\ \mathcal{J}_{\text{MFG}}(v,\rho) \overset{\text{def}}{=} \int_0^1 \int_{\mathbb{R}^d} L\left(x, v(x,t)\right) \rho(x,t) dx dt + \int_0^1 \mathcal{F}(\rho(\cdot,t)) dt + \mathcal{G}(\rho(\cdot,1))$$

$$\text{subject to} \quad \partial_t \rho(x,t) + \nabla \cdot (\rho(x,t) v(x,t)) = 0, \quad \rho(x,0) = \rho_0(x),$$

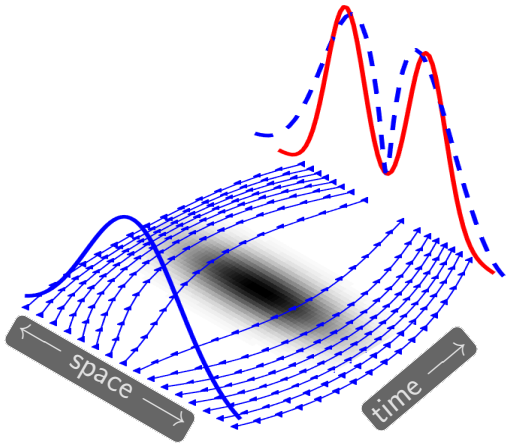
Use running costs $\mathcal{F}$ to model, e.g.,

- congestion

$$\mathcal{F}_{\text{E}}(\rho) = \int_{\mathbb{R}^d} \rho(x) \log(\rho(x)) dx$$

- spatio-temporal preference

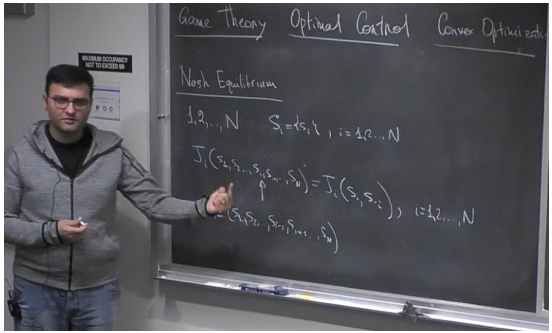
$$\mathcal{F}_{\text{P}}(\rho) = \int_{\mathbb{R}^d} Q(x) \rho(x,t) dx$$



More To Watch

Levon Nurbekyan @ IPAM Opening Workshop

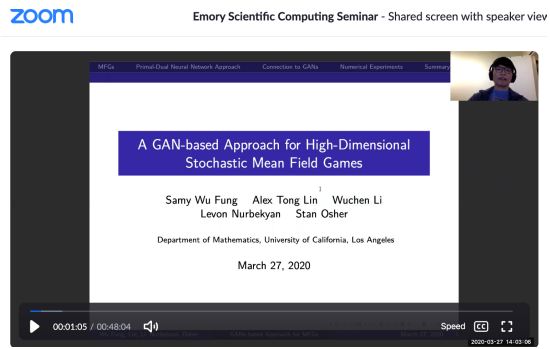
Computational methods for mean-field games



https://bit.ly/3cELBmW

Samy Wu Fung @ Emory Scientific Computing Seminar

A GAN-based Approach for High-Dimensional Stochastic Mean Field Games



https://bit.ly/2TcqvVp

Optimal Transport $\rightarrow$ Continuous Normalizing Flows

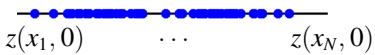
Continuous Normalizing Flows (CNF)

Likelihood Maximization

Given samples $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$, find a velocity v that maximizes the likelihood of the samples w.r.t. the push-forward of the standard normal distribution ρ_1, i.e.,

$$\begin{aligned} \text{maximize}_{v,z} \quad & \frac{1}{N}\sum_{k=1}^{N} \rho_1(z(x_k,1)) \cdot \det \nabla(z(x_k,1)) \\ \text{subject to} \quad & \partial_t z(x_k,t) = v(z(x_k,t),t), \end{aligned}$$

with $z(x_k,0) = x_k$ for all k.



W Grathwohl et al.
FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models. *arXiv*, 2018.

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$$\text{subject to} \quad \partial_t \begin{pmatrix} z(x_k,s) \\ l(x_k,s) \end{pmatrix} = \begin{pmatrix} v(z(x_k,s),s) \\ \operatorname{trace}(\nabla v(z(x_k,s),s)) \end{pmatrix}$$

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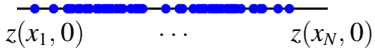

Recall: $l(x_k,1) = \log\det(\nabla z(x_k,1))$

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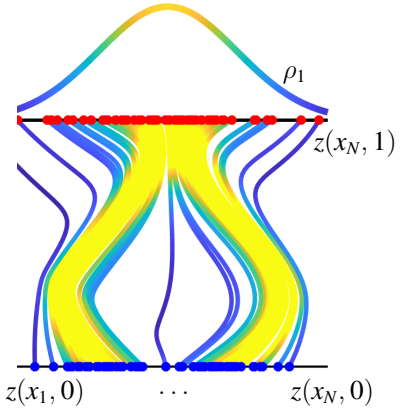

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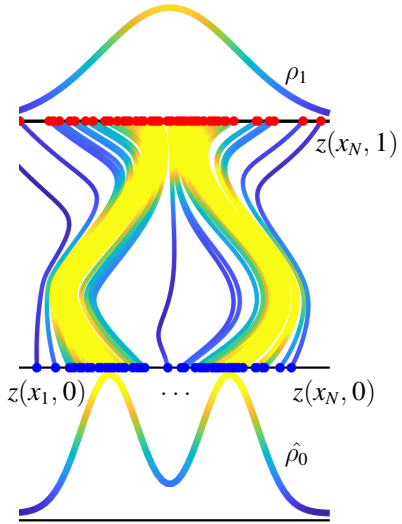



D. Onken S. Wu Fung X. Li

OT-Regularized Continuous Normalizing Flow

OT-Flow: Regularized Continuous Normalizing Flow

Given samples $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$, find the value function Φ such that the flow given by $v = -\nabla\Phi$ maximizes the likelihood of the samples w.r.t. the standard normal distribution ρ_1, i.e.,

$$\min_{v,z} \frac{1}{N}\sum_{k=1}^{N}\left[\frac{1}{2}\|z(x_k,1)\|^2 - l(x_k,1) + \beta_1 c_{\mathrm{L}}(x_k,1) + \beta_2 c_{\mathrm{H}}(x_k,1)\right]$$

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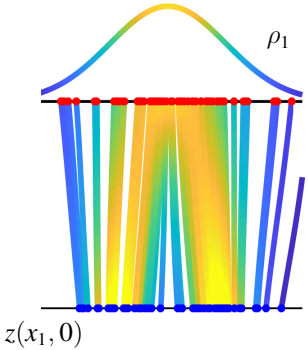

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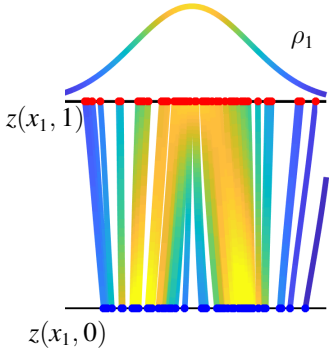

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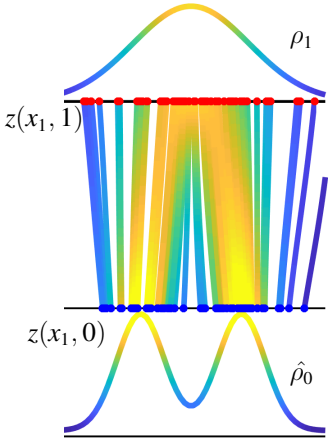

- provides uniqueness
- more efficient time integration

L Yang, GE Karniadakis
Potential Flow Generator with L_2 OT Regularity for Generative Models.
arXiv:1908.11462v1, 2018.

L Zhang, Weinan E, L Wang
Monge-Ampère Flow for Generative Modeling, *arXiv:1809.10188v1*, 2018.

C Finlay, JH Jacobsen, L Nurbekyan, AM Oberman
How to train your neural ODE, *arXiv:2002.02798*, 2020.

Trace Computation: Runtime and Accuracy

- Exact computation with automatic differentiation (AD)

$$\operatorname{trace}(\nabla v(x)) = \sum_{i=1}^{d} e_i^\top (\nabla v(x)^\top e_i)$$

☀️ exact 🌨️ $\mathcal{O}(m \cdot d^2)$ FLOPS

- trace estimator with AD

$$\begin{aligned}\operatorname{trace}(\nabla v(x)) &= \mathbb{E}_w \left[w^\top (\nabla v(x)^\top w) \right] \\ &\approx \frac{1}{S} \sum_{k=1}^{S} (w_k)^\top (\nabla v(x)^\top w_k)\end{aligned}$$

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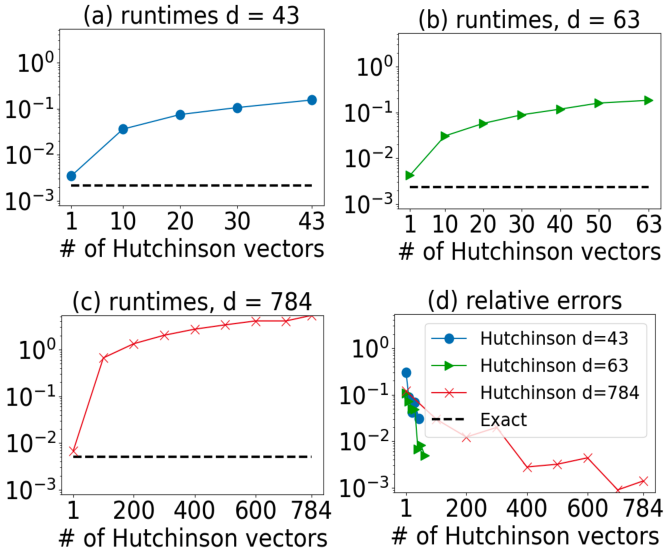


Trace Computation: Runtime and Accuracy

- Exact computation with automatic differentiation (AD)

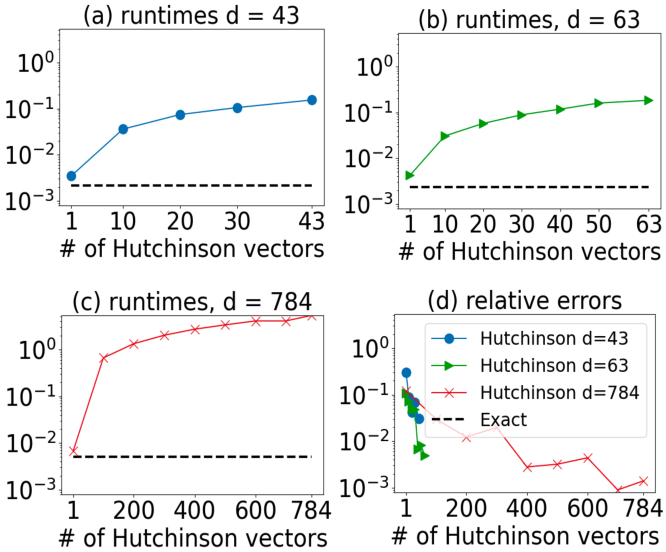
$$\text{trace}(\nabla v(x)) = \sum_{i=1}^{d} e_i^\top (\nabla v(x)^\top e_i)$$

☀️ exact 🌧️ $\mathcal{O}(m \cdot d^2)$ FLOPS

- trace estimator with AD

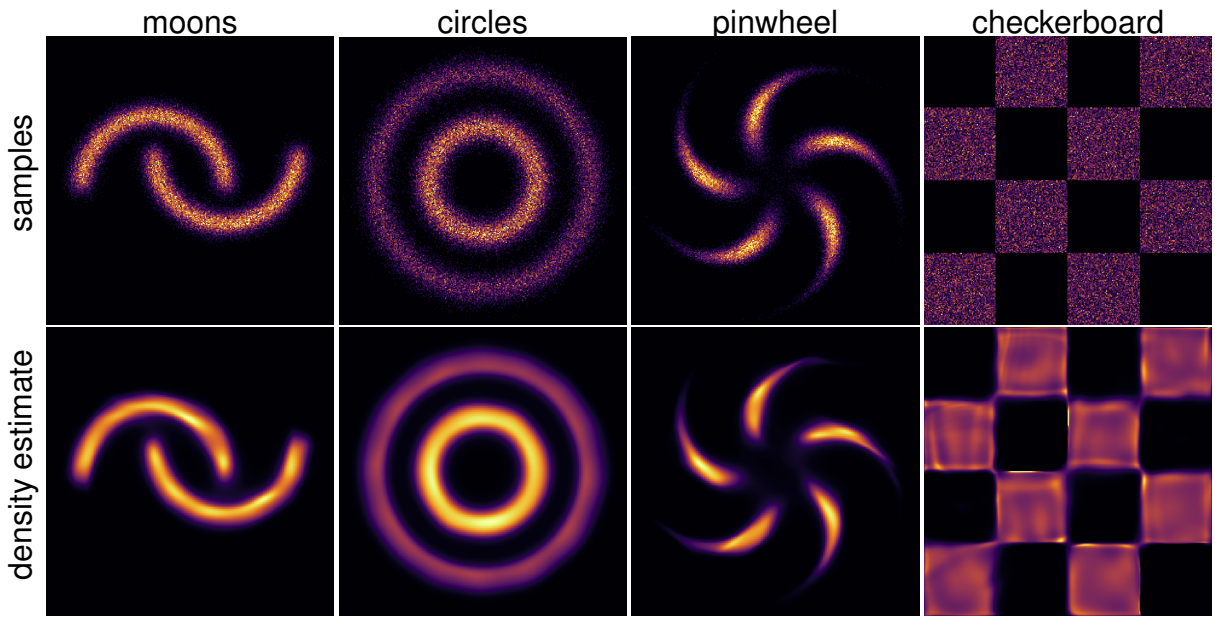
$$\text{trace}(\nabla v(x)) = \mathbb{E}_w \left[w^\top (\nabla v(x)^\top w) \right]$$
$$\approx \frac{1}{S} \sum_{k=1}^{S} (w_k)^\top (\nabla v(x)^\top w_k)$$

🌧️ inexact ☀️ $\mathcal{O}(m \cdot S \cdot d)$ FLOPS

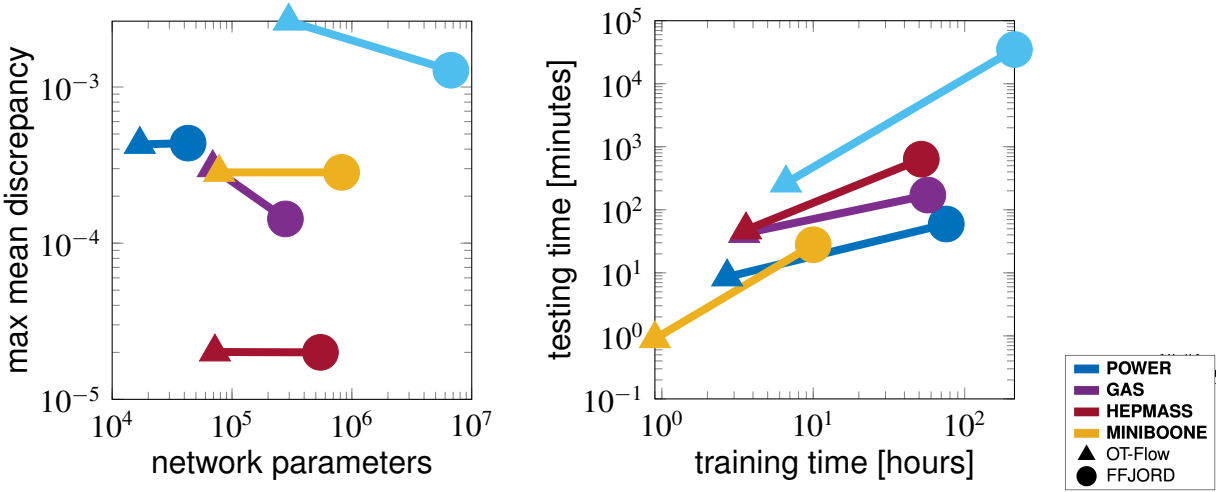


OT-Flow: exact trace computation (highly parallel) using $\mathcal{O}(m^2 \cdot d)$ FLOPS.

OT-Flow: Two-Dimensional Examples



OT-Flow vs. FFJORD: Comparison for UCI Datasets

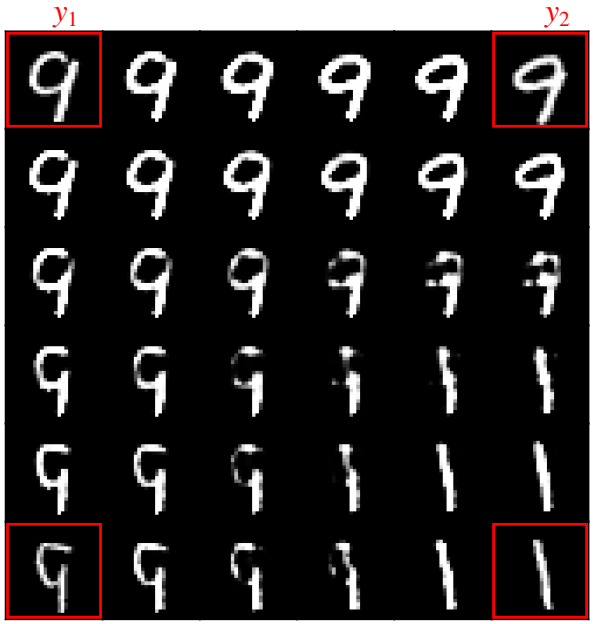


- FFJORD slightly superior to OT-Flow w.r.t. MMD
- FFJORD needs between 2× and 22× more weights
- Speed up of OT-Flow: between 11× and 32× (training) and 4× and 131× (testing)

OT-Flow Example: Generative Modeling MNIST

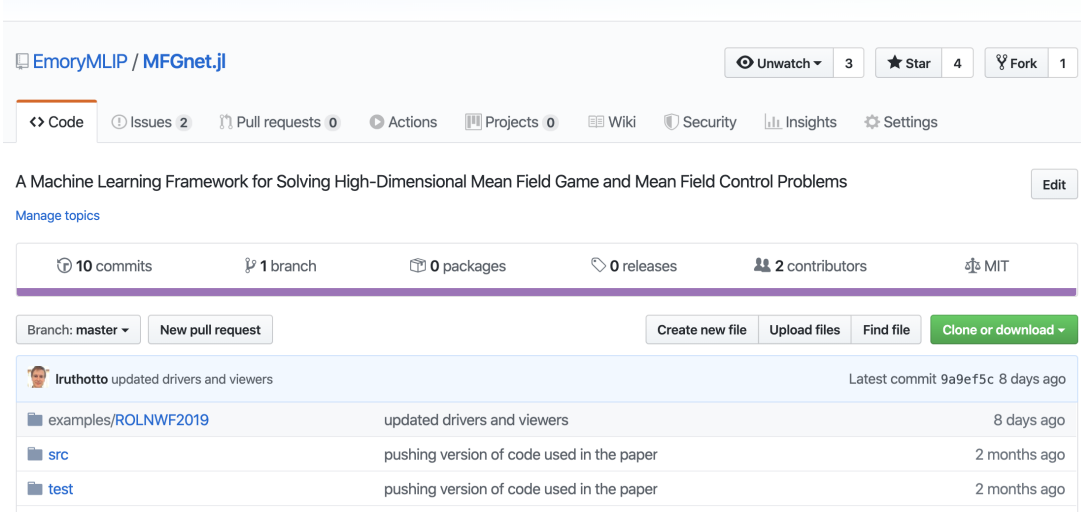
- let $y_1, y_2, \ldots \in \mathbb{R}^{768}$ MNIST images
- train encoder $E : \mathbb{R}^{784} \to \mathbb{R}^{128}$ and decoder $D : \mathbb{R}^{128} \to \mathbb{R}^{784}$ s.t. $D(E(y)) \approx y$
- latent space representation of data $x_j = E(y_j)$ for all j.
- train OT-Flow f that maps $\{x_j\}_j$ to $\rho_1 \sim \mathcal{N}(0, I_{128})$
- interpolate between two images y_1, y_2 in latent space and get new image

$$y(\lambda) = D(f^{-1}(\lambda f(E(y_1)) + (1-\lambda) f(E(y_2))))$$



Conclusions

MFGnet.jl - Julia Package



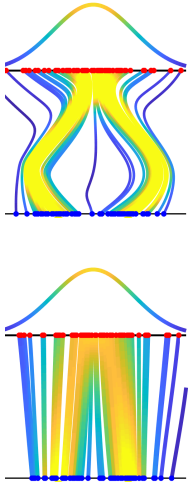
https://github.com/EmoryMLIP/MFGnet.jl

Efficient pytorch implementation for CNF:
https://github.com/EmoryMLIP/OT-Flow.py

Σ: Machine Learning meets Optimal Transport

Machine Learning $\rightarrow$ Optimal Transport

- ML attractive for **high-dimensional** PDEs, control, ...
- MFGnet: mesh-free solver for variational problem and combine...
  - microscopic: Lagrangian method for continuity and HJB eqs.
  - macroscopic: variational problem, new penalties for HJB eq.
- **details matter: models, numerics, architecture, training, ...**
- **surprise: ML solution competitive to convex programming**



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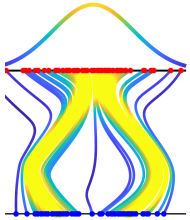
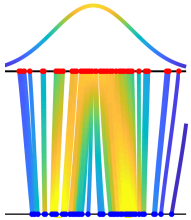


Optimal Transport → Continuous Normalizing Flows

- OT regularization: well-posed simplifies time integration
- discretize-then-optimize + HJB penalty → very few time steps
- **don't take chances: use exact trace computation**
- **OT-Flow speeds up training and testing by ≈ 10x**



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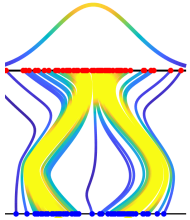

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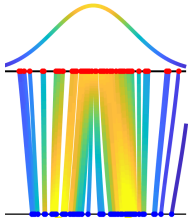

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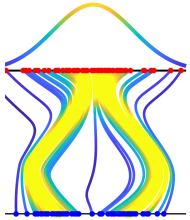

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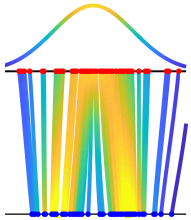

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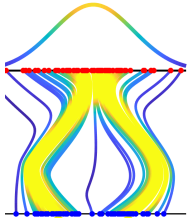

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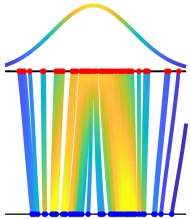

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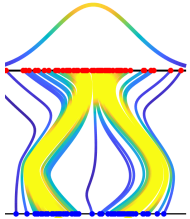

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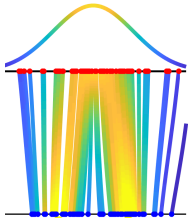

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